

Taurocyamine

543-18-0 | DTXSID10202654

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 7.26

Global applicability domain: Outside

Local applicability domain index: 1.46e-01

Confidence level: 4.31e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>4-Hydroxybenzoic acid</div> <div>Measured: 8.08</div> <div>Predicted: 7.78</div>	<div>Image not found</div> <div>Salicylic acid</div> <div>Measured: 7.44</div> <div>Predicted: 7.60</div>	<div>Image not found</div> <div>Methylparaben</div> <div>Measured: 8.57</div> <div>Predicted: 7.06</div>
<div>Image not found</div> <div>1-Octanol</div> <div>Measured: 6.03</div> <div>Predicted: 5.95</div>	<div>Image not found</div> <div>Cyclohexanol</div> <div>Measured: 5.18</div> <div>Predicted: 4.72</div>	